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Journal of Alloys and Compounds 380 (2004) 84–88

Journal of
ALLOYS
AND COMPOUNDS

www.elsevier.com/locate/jallcom

Crystal field and magnetic ordering in the Haldane-chain compound $\text{Er}_2\text{BaNiO}_5$ as studied by optical spectroscopy

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Abstract

High-resolution absorption spectra of the chain compound $\text{Er}_2\text{BaNiO}_5$ were measured in a wide range of frequencies (6000–20,000 cm^{-1}) and temperatures (2.5–300 K). Energies of 38 crystal-field levels of Er^{3+} in a paramagnetic $\text{Er}_2\text{BaNiO}_5$ were determined. Exchange splittings of crystal-field levels in the antiferromagnetically ordered state ($T_N = 34$ K) were measured. Crystal-field calculations were performed and the obtained wave functions were used to calculate the temperature dependence of the magnetic susceptibility to be compared with the detailed experimental dependence measured in this work.

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Keywords: Absorption; Er^{3+} ; Crystal-field calculations; Phase transition; Exchange splittings

1. Introduction

The nickelates R_2BaNiO_5 with $\text{R} = \text{Y}, \text{Nd–Gd}, \text{Dy–Tm}$ feature antiferromagnetic (AF) $S = 1$ Ni^{2+} chains interconnected by either nonmagnetic ($\text{R} = \text{Y}$) or magnetic ($\text{R} = \text{rare earth}$) ions. Recently, they have attracted a considerable attention as model systems to study the one-dimensional (1D) magnetism, 1D to 3D crossover, the magnetic excitations of an integer-spin AF chains (Haldane chains) and the interaction of these excitations with the electronic excitations of the rare-earth subsystem (see, e.g. [1] and the references therein). To continue these studies, it is essential to know the energies and the wave functions of the crystal-field levels for the rare-earth R^{3+} ions in R_2BaNiO_5 compounds. Almost no such information was available up till now. So, we decided to undertake a systematic study of the crystal-field effects in R_2BaNiO_5 . The present work on $\text{Er}_2\text{BaNiO}_5$ is the first step in this direction.

Neutron scattering [2] and spectroscopic [3] experiments revealed a magnetic ordering of $\text{Er}_2\text{BaNiO}_5$ at $T_N \approx 34$ K.

As followed from the inelastic neutron scattering data at $T = 1.7$ K, both nickel and erbium ordered magnetic moments are directed antiferromagnetically along the crystallographic axis a parallel to the direction of the Ni–O–Ni chains [2]. The magnetic susceptibility curve $\chi(T)$ did not display, however, any peculiarity at T_N , but exhibited a well-defined maximum at the much lower temperature, $T_m = 15$ K [4,3]. This maximum was first attributed to a magnetic phase transition within the Er magnetic subsystem [2]. However, in our earlier spectroscopic study of the magnetic ordering in $\text{Er}_2\text{BaNiO}_5$ [3] we have shown qualitatively that the maximum at 15 K in the $\chi(T)$ curve can be explained by a depopulation of the upper component of the Er ground state Kramers doublet split by the exchange interaction in a magnetically ordered state. This conclusion was based on the spectroscopically measured ground state splitting and on a preliminary information obtained from the measured $^4\text{I}_{15/2} \rightarrow ^4\text{I}_{13/2}$ spectra [3], namely, that the first excited crystal-field level lies not lower than at 35 cm^{-1} .

In this work, we study the temperature-dependent absorption spectra of many optical transitions of Er^{3+} in $\text{Er}_2\text{BaNiO}_5$ and find the energies of all the crystal-field (CF) levels for the ground state manifold $^4\text{I}_{15/2}$ as well as for

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